

# Tuning Assembly Size in Peptide-Based Supramolecular Polymers by Modulation of Subunit Association Affinity

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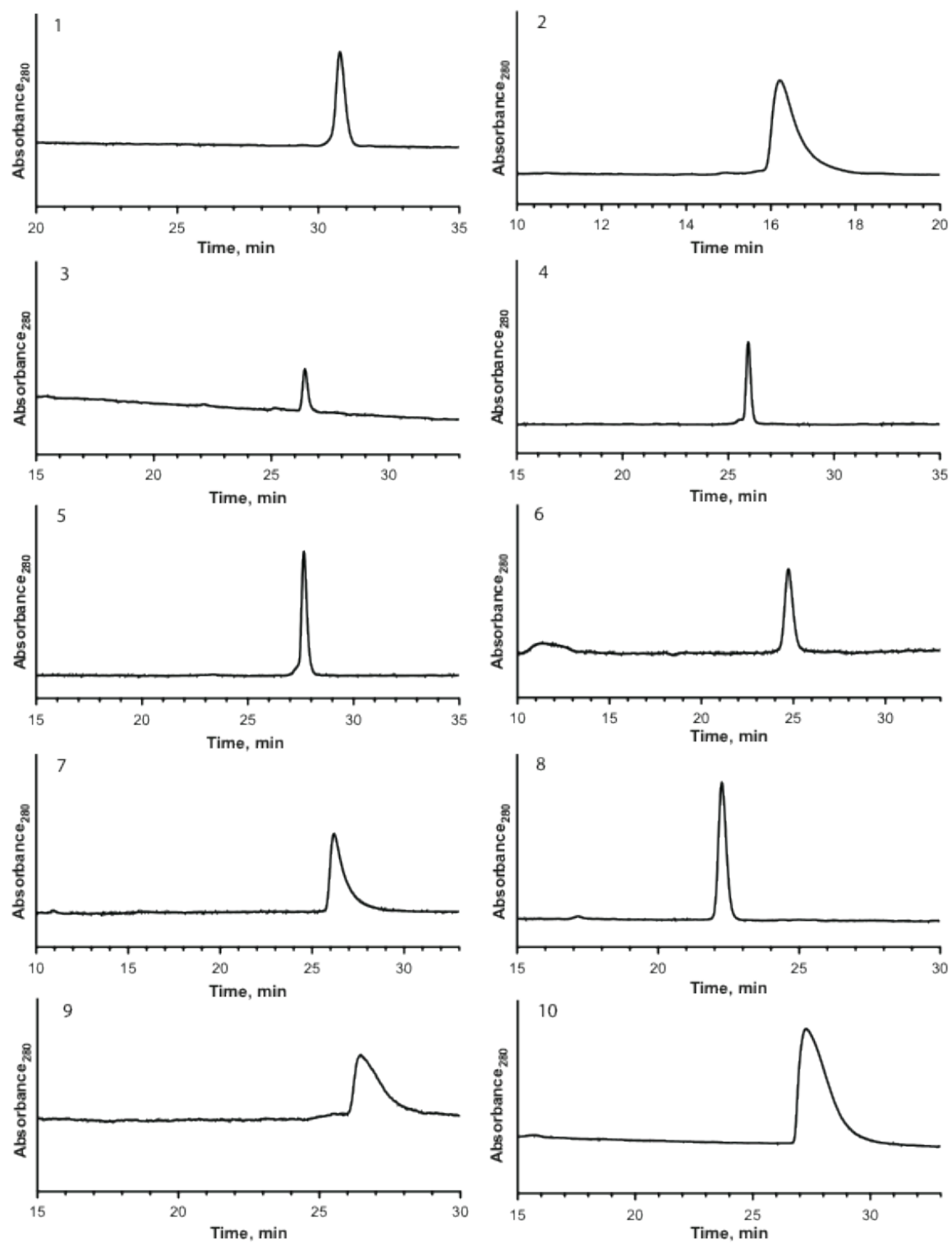
## SUPPORTING INFORMATION

**Table S1.** MALDI-TOF data for the synthetic peptides and subunits.

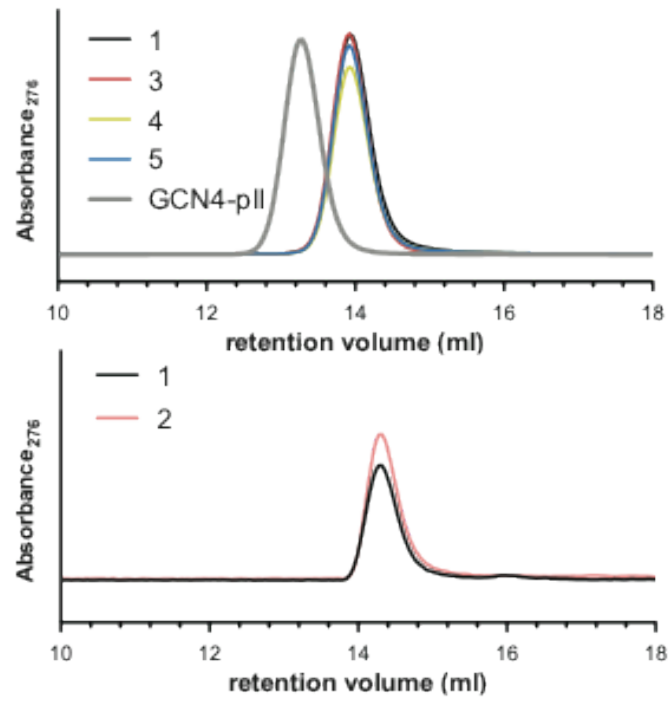
#	[M + H] <sup>+</sup> <i>m/z</i> (avg.)	
	Calculated	Observed
<b>1</b>	4038.7	4036.9
<b>2</b>	4024.6	4022.4
<b>3</b>	4052.7	4051.2
<b>4</b>	4066.7	4065.8
<b>5</b>	4080.7	4079.7
<b>6</b>	4054.7	4054.7
<b>7</b>	4040.7	4037.2
<b>8</b>	4068.7	4067.1
<b>9</b>	4082.7	4081.1
<b>10</b>	4096.8	4095.4
<b>6s</b>	8274.6	8274.7
<b>7s</b>	8246.6	8243.7
<b>8s</b>	8302.7	8297.6
<b>9s</b>	8330.7	8325.2
<b>10s</b>	8358.7	8355.8

**Table S2.** X-ray crystallography collection and refinement statistics.

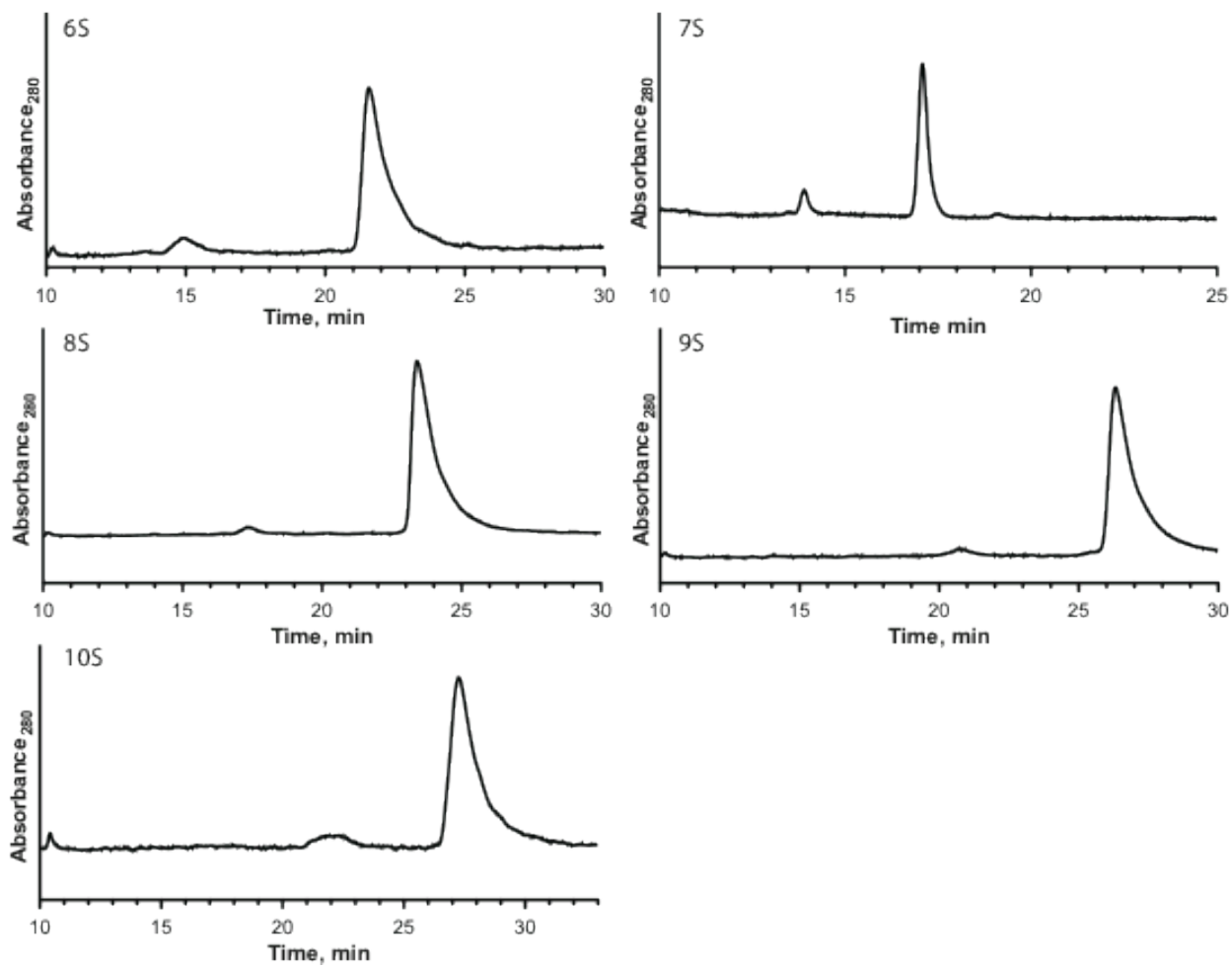
	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
<b>PDB ID</b>	<b>4NIZ</b>	<b>4NJ0</b>	<b>4NJ1</b>	<b>4NJ2</b>
<b>Space Group</b>	<b>C2</b>	<b>C2</b>	<b>C2</b>	<b>C2</b>
<b>Unit Cell</b>				
<i>a</i> , <i>b</i> , <i>c</i> (Å)	82.3, 30.1, 27.8	83.2, 30.4, 27.8	83.4, 30.5, 27.9	39.4, 36.7, 47.6
<i>α</i> , <i>β</i> , <i>γ</i> (°)	90, 101.3, 90	90, 102.0, 90	90, 102.1, 90	90, 104.8, 90
<b>Data Collection</b>				
Resolution Range (Å)	28.23–2.00 (2.07–2.00)	40.69–1.90 (1.97–1.90)	28.55–2.00 (2.07–2.00)	24.89–2.20 (2.28–2.20)
Total Reflections	15493	17995	11581	10822
Unique Reflections	4580	5462	4582	3367
Completeness	98.7 (94.8)	99.3 (97.6)	96.2 (86.5)	98.5 (96.5)
Redundancy	3.4 (2.1)	3.3 (2.2)	2.5 (1.7)	3.2 (3.3)
<i>I</i> / <i>σ</i>	30.3 (4.7)	20.4 (2.2)	28.3 (4.8)	8.2 (1.8)
R <sub>merge</sub>	0.03 (0.09)	0.05 (0.26)	0.03 (0.09)	0.09 (0.29)
<b>Refinement</b>				
Resolution (Å)	27.31–2.00	27.18–1.90	27.31–2.00	24.98–2.20
R (%)	21.2	25.9	24.2	24.8
R <sub>free</sub> (%)	24.3	28.3	25.5	30.0
Average B factor (Å <sup>2</sup> )	20.1	28.8	25.7	28.6
<b>RMSD</b>				
Bonds (Å)	0.005	0.003	0.002	0.01
Angles (°)	0.62	0.65	0.33	1.3



**Figure S1.** Analytical HPLC chromatograms of the purified peptides **1-10**.



**Figure S2.** Gel permeation chromatography of the subunits confirming the dimeric oligomerization state.



**Figure S3.** Analytical HPLC chromatograms of the purified subunits **6s-10s**